

Ethyl hydroperoxide
3031-74-1 | DTXSID70184402

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4.97 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.05e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Acetic acid</div> <div>Measured: 1.00</div> <div>Predicted: 2.40</div>	<div>Image not found</div> <div>Acrylamide</div> <div>Measured: 50.1</div> <div>Predicted: 16.7</div>	<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 3.02</div> <div>Predicted: 4.69</div>
<div>Image not found</div> <div>Acetamide</div> <div>Measured: 5.01</div> <div>Predicted: 4.44</div>	<div>Image not found</div> <div>Thioacetamide</div> <div>Measured: 6.03</div> <div>Predicted: 6.43</div>	